Hexachloropropene

1888-71-7 🛭	TXSID7062039

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 455 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.53e-01

Confidence level: 7.04e-01

Nearest Neighbors from the Training Set

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Tetrachloroethylene Measured: 251 Predicted: 170

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Hexachlorobenzene Measured: 5500 Predicted: 6740

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1,2-Dibromo-3-chloropropane **Measured:** 70.8

Measured: 70.8 Predicted: 84.1

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1,1,2,2-Tetrachloroethane

Measured: 79.4 Predicted: 77.8

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Pentachlorobenzene Measured: 3160 Predicted: 5490